Laboratory Name: Sandia National Laboratories, CA
B&R Code: KC020101

FWP and subtask under FWP:
FWP Dynamics and Structure of Interfaces and Dislocations
Subtask: Metallic Interfaces and Dislocations

FWP Number: SCW604

Program Scope:
This sub-program seeks to establish the basic principles that control the structure and behavior of internal interfaces. We concentrate on metallic interfaces, including both grain boundaries and heterophase interfaces, with a central goal of determining how the incompatibilities and discontinuities that arise at such interfaces are accommodated and what the implications of these relaxations are on the behavior and properties of the interface. One key to establishing this connection is in understanding the nature of interfacial defects. Just as bulk crystal behavior is dominated by the properties of lattice defects, one anticipates that interfacial processes are similarly controlled by the properties of point (e.g., vacancies and impurities) and extended defects (steps, dislocations, and junctions) present on the interface. A second key is in establishing how these defects interact with each other and with the interface itself. For instance, in real polycrystalline solids, boundaries of finite length terminate at junctions with other boundaries, and even a single boundary often deviates from the simple planar ideal, forming an array of atomic-scale steps or breaking up into an array of larger scale facets. Finally, it is important to understand how interfaces are controlled by composition. To address such questions, we combine detailed experimental observations using atomic-resolution microscopies with comprehensive theory and modeling, encompassing electronic structure, atomistic, and continuum simulations. We see a crucial challenge in exploring what controls the *three-dimensional* evolution of interfaces. Thus, we are applying new imaging techniques, such as atom probe tomography, and developing new theoretical approaches to provide fundamental insights into this important class of problems. Throughout, our approach is to employ both experimental and theoretical tools to obtain a basic scientific understanding of the fundamental structural elements, interactions, and excitations that govern interfacial behavior. Ultimately, a comprehensive picture of how these seemingly disparate structural elements work in concert will improve our ability to predict and control a diverse range of interface mediated materials processes.

Major Program Achievements (over duration of support):
Key accomplishments include: Explanation of size dependence for shape distributions in embedded metallic precipitates; Discovery of structural phase transition for the {112} twin boundary; Quantitative analysis of size effects on the structure of grain boundary; Discovery of grain boundary interactions through extended stacking fault formation; Analysis of defaceting grain boundary transition and discovery of new faceting mechanism; Discovery of mechanism for heterophase misfit accommodation through an interfacial reconstruction.

Program Impact: Have developed a quantitative understanding based on coupling simulation and microscopy of grain boundary structures.

Interactions:
Uli Dahmen, NCEM/LBL; C.B. Carter, University of Minnesota; Y. Mishin, George Mason University; I. Daruka, University of Debrecen, Hungary; A. Voter, LANL; S.M. Foiles, SNL/NM; R.C. Pond, Univ. of Liverpool, UK.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
D.L. Medlin: Chair 2006 Gordon Research Conference on Physical Metallurgy.
J.C. Hamilton: Organizer of symposium at the Fall 2005 Meeting of the MRS

Personnel Commitments for FY2006 to Nearest +/- 10%:
D.L. Medlin (40%), J.C. Hamilton (30%), E. Marquis (40%).

Authorized Budget (BA) for FY04, FY05, FY2006:
FY04 BA $385K **FY05 BA $**368K **FY06 BA $**340K

Laboratory Name: Sandia National Laboratories, CA
B&R Code: KC020101

FWP and subtask under FWP:
FWP Dynamics and Structure of Interfaces and Dislocations
Subtask: Surface Dynamics

FWP Number: SCW604

Program Scope:
The goal of this project is to quantify the fundamental atomic processes governing the dynamics of surface structure and morphology. We use state-of-the-art microscopy (low-energy electron microscopy and scanning tunneling microscopy) to measure, often in real time, the time evolution of surface structure on nanometer length scales. We use these measurements to write down precise equations of motion to describe the observed time dependence and then relate these equations of motion to atomic processes. We have used this general approach on a variety of different problems in surface science. This work has often revealed unanticipated mechanisms of surface evolution. We currently emphasize five focus areas: 1) film wetting and de-wetting, 2) mass exchange between the bulk and surface, 3) surface self-assembly, 4) oxide surfaces and metal oxidation, and (5) surface alloying. The goal of future work is to apply our approach to increasingly complicated material systems and further develop the conceptual framework needed to account for our observations. The ultimate goal is to provide the groundwork for quantitative predictions needed to engineer surface properties.

Major Program Achievements (over duration of support):
Key accomplishments include: determining the atomic-scale dynamics governing self-assembly of nanoscale patterns on surfaces; real-time observations and atomistic interpretation of the evolution of thin-film microstructure (e.g., twin-boundary motion); quantitative measurements of dislocation dynamics in thin film and their relationships to surface morphology; discovery of new surface growth modes due to surface alloying; measurement of the thermodynamic stability of supported oxide nanostructures; discovery of new fundamental atomic mechanisms for the dynamics of surface morphology. In particular, we have determined the quantitative link between bulk vacancy formation and transport to surface smoothing and the role of substrate atomic steps in the de-wetting of thin metal films.

Program Impact:
By a combination of experiment and theory, we are among the first to be able to account quantitatively for the kinetic processes that determine the nanoscale surface structure. There is considerable recent interest in the materials science of nanoscale features on surfaces because of their possible applications in the development of new energy technologies. For example, understanding bulk-surface exchange is important for the development of hydrogen storage materials, and metal oxide surfaces are important industrial catalysts.

Interactions:
J. de la Figuera (Univ. Autónoma de Madrid); R. Q. Hwang (BNL); P. Hou, Andreas Schmid (LBNL); C. B. Carter (Univ. Minnesota); S. Chiang (UC Davis); J. B. Hannon (IBM Research); G. L. Kellogg, P. J Feibelman, B. S. Swartzentruber (SNL/NM); F. Besenbacher (Aarhus).

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
23 Publications (2004-2006), including 2 articles in Science, 6 articles in Physical Review Letters, and one article in Nanoletters. 2001 MRS Medal (Bartelt); 2001 Nottingham Prize (Thayer). Editorial boards of Physical Review Letters and Surface Science (Bartelt) and Materials & Engineering Reports (McCarty).

Personnel Commitments for FY2006 to Nearest +/- 10%:
N. C. Bartelt (100%), K. F. McCarty (70%), K. Thuermer (70%), J. C. Hamilton (20%), J. P. Pierce (post-doc) (100%).

Authorized Budget (BA) for FY04, FY05, FY2006:
FY04 BA $1150k ($770K/349K) **FY05 BA $**1150K **FY06 BA** $1034K
Note: in FY05, FWP SCW1550 ("Oxide Surfaces and their Interactions with Metals") was combined with SCW604 subtask on "Surface Dynamics". The above budget numbers show the distribution between these two projects.

Laboratory Name: Sandia National Laboratories, CA
B&R Code: KC020101

FWP and subtask under FWP:
FWP Dynamics and Structure of Interfaces and Dislocations
Subtask: Alloying at Surfaces and Interfaces

FWP Number: SCW604

Program Scope:
The Alloying at Surfaces and Interfaces program at Sandia, California is focused on the development, validation and application of computational methods that can be used to explain and predict structural, mechanical, and thermodynamic properties of materials. We use and develop first-principles atomic scale and continuum methods. A current focus of the program is on using these techniques to understand the mechanisms of alloying and de-alloying. The ultimate goal of the program is to uncover fundamental concepts that can be applied to understanding the structure, behavior and processing of alloys. The main research areas are: (i) atomistic mechanisms that govern ultrathin film and surface alloy formation; (ii) role of dislocations during phase separation of bulk alloys; (iii) role of H in energetics and kinetics of alloy formation and segregation at surfaces and interfaces; (iv) development and implementation of the self-consistent GW method; and (v) free energy in bulk and surface alloys.

Major Program Achievements (over duration of support):
Key accomplishments include: Development of continuum models to study the influence of dislocations on phase separation in binary alloys; Role of activation energies for surface and bulk intermixing in causing composition gradients during heteroepitaxy of Au on W(110), Pd on Ru(0001) and Ge on Si(001); Effect of H on the formation of near surface alloys of transition metals with Al and Mg surfaces; Development of anisotropic elasticity approach for self-assembly at solid surfaces, providing theoretical explanation for the unusual orientation of stripes in the PbCu system; Development of the self-consistent GW method, and applications to a broad range of materials; Development of first principles tool to determine vibrational entropies and test on H containing materials.

Program Impact: Has expanded our understanding of the mechanisms of solute stability in alloys and their implications to alloy behavior, and our understanding of the mechanisms of alloying and de-alloying. Provided a new, accurate method for calculating the electronic structure of a wide range of materials. Provided insight into role of transition metals in improving the rates of H_2 sorption in complex hydrides.

Interactions:
Dr. Mikko Haataja (Princeton Materials Institute)
Dr. B. S. Swartzentruber (Sandia National Laboratories, Albuquerque, New Mexico)
Dr. J. B. Hannon (IBM T.J. Watson Research Center, New York)
Dr. J. J. Hoyt (Sandia National Laboratories, Albuquerque, New Mexico)
Dr. John Hamilton (Sandia National Laboratories)
Dr. Norman Bartelt (Sandia National Laboratories)
Dr. Andreas Schmidt (Lawrence Berkeley National Laboratories)
Dr. Nicholas Rougemaille (Lawrence Berkeley National Laboratories)
Dr. Mark van Schilfgaarde (Arizona State University)

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
R. Stumpf : co-organizer of a symposium on advanced H storage materials at the Fall 2004 MRS meeting.
F. Léonard: invited speaker and panelist at Nanocommerce conference, and part of advisory committee for joint chemical/semiconductor industry research for National Nanotechnology Initiative. S. Faleev: invited speaker at conference on “Quantum Transport and Non-Adiabatic Electron Evolution from First Principles Approaches.”

Personnel Commitments for FY2006 to Nearest +/- 10%:
R. Stumpf (35%), F. Léonard (50%), S. Faleev (50%) (Limited-Term).

Authorized Budget (BA) for FY04, FY05, FY2006:
FY04 BA $349K **FY05 BA $**333K **FY06 BA $**344K

Sandia National Laboratories/NM

Annual BES/DMS&E One-Page Summaries

Laboratory Name: Sandia National Labs/NM
B&R Code: KC020102

FWP: Mechanics of Small Length Scales

FWP Number: SCW 93221

Program Scope: The basis of this program is the study of mechanical response down to the nanoscale in order to obtain atom-level control and understanding of the elastic and plastic deformation of bulk and nanostructured materials, thermal evolution of micro- and nanostructure, physics of mechanical dissipation/transformation of mechanical energy/collective behavior of mechanically-coupled systems, and strain-driven growth/morphological evolution/nanostructure synthesis.

Major Program Achievements (over duration of support): Collectively, this work spans length scales ranging from single atomic defect mechanical relaxation up to microscale morphological evolution. We have brought new understanding to such diverse mechanical phenomena as plastic deformation in nano-structured materials, strain-controlled ordered nanostructure self-assembly, and atomic-scale defect relaxation in nanoresonators. Specific program highlights include:

Nanostructured Materials: **Direct *in situ* TEM evidence for grain-boundary deformation processes and large lattice strains, with simultaneous dislocation propagation, in nano-grain Ni. **Identified thermal instability of nanocrystalline Ni leading to abnormal grain growth (combined with theoretical study, below). **Developed new understanding of origin of tensile stress in metal films due to island coalescence.

Theory of Microstructures: ** First physically-based model for nucleation of recrystallization from deformation substructure. **New MD method for computing mobility of flat grain boundaries with/without solute. **First simulations of abnormal nanocrystal growth due to geometric/ crystallographic gradients. **First proof that genetic algorithms exceed simulated annealing for structure optimization. **New scaling theory for 2D/3D grain boundary networks proving R-curve behavior is intrinsic to polycrystals.

Advanced Growth: **Developed novel real-time diagnostics for thin film growth: energy dispersive x-ray reflectivity/multibeam optical stress sensor/light scattering spectroscopy. **Quantitative understanding of morphological evolution of heteroepitaxial SiGe quantum dot arrays. **Kinetically-controlled heteroepitaxial self-assembly to produce ordered functional nanostructures. **Identified fracture energetics and slip processes in strained III-nitride heterostructures.

Dissipation and Coupled Systems: **Developed new capability for measuring defect-related internal dissipation in micro- and nanoresonators. **First measurements of defect distributions in diamond resonators. **Developed MD method for identifying atomistics of defect-related internal dissipation.

Plasma Crystals: **First measurements of the ion wakefield induced binding potential in 3D crystals. **First measurements of the electric field distribution on particles immersed in a plasma. **Developed new analysis technique to directly determine particle-particle interaction potential in 2D plasma crystals.

Program impact: Research has led to new understanding of mechanisms of strengthening materials via nanostructuring, enabling development of high performance materials. The new computational methods enable the robust prediction of the evolution of micro/nanostructure in materials, enabling design and performance prediction of new materials. The novel real-time growth diagnostics permit new understanding of the energetics/kinetics of heteroepitaxial self-assembly, leading to the controlled synthesis of nanostructures for mechanical/optical/electronic applications. Experiment and theory of internal dissipation provides understanding of energy transformation in micro/nanomechanical systems for nanotechnology.

Interactions: On-going collaborations with 24 institutions including government and universities.

Recognitions, Honors and Awards: Floro: MRS BoD 02-04, MRS Public Outreach Chr, MRS Mtg Chr 01 **Follstaedt**: R&D100 04. **Hebner**: AVS Plasma Prize, AVS Fellow. **Holm**: NMAB 04-07, TMS BoD 04-07, THERMEC 06 Intl Sci Comm, PRICM5 org 04, NWU John Dorn Lecturer (2005.
Invited presentations since 1995: 118 Archival publications since 1995: 123

Personnel Commitments for FY2006 to Nearest +/- 10%: Floro 90%, Follstaedt 30%, Friedmann 20%, Hearne 20%, Hebner 10%, Holm 30%, Knapp 20%, Modine 10%, Pan 10%, Sullivan 30%, Wendt 10%

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA: $1,227K **FY05 BA:** $1,030K **FY06 BA:** $1,030K

Laboratory Name: Sandia National Labs/NM
B&R Code: KC020103

FWP: Atomic Scale Surface Phenomena

FWP Number: SCW 93219

Program Scope: Our goal is to develop an atomic-scale understanding of physical and chemical processes at surfaces and interfaces in three major thrust areas: (1) adhesion and wetting, (2) localized corrosion, and (3) surface nanostructure formation. Our approach is to combine state-of-the-art experimental probes with modern theoretical techniques to produce the scientific understanding necessary to predict and control macroscopic materials properties.

Major Program Achievements (over duration of support): (1) We invented the interfacial force microscope (IFM), the world's first (and only) scanning probe instrument that can measure normal and lateral forces simultaneously throughout the entire attractive/repulsive interaction regime. We achieved an understanding of two-stage plasticity in nanoscale contacts, yield strength softening by surface defects, interphase mechanical properties in nanocomposite materials, origins of friction and energy dissipation in self-assembled alkanethiol monolayers, and the surprising behavior of liquids near solid surfaces. (2) We discovered that when aluminum is exposed to water, nanoscale open pores develop at the oxide surface and these pores are linked to aluminum pitting in the presence of aggressive species. We showed that these pores initiate as voids at the oxide/metal interface and grow towards the surface, with the highest concentrations developing at high-curvature surfaces. We recently found the first evidence of locally induced oxidation of the copper surface in naturally aerated acidic media. (3) We discovered important new mechanisms for dynamic surface processes including a remarkable self-assembly process for Pb atoms on Cu surfaces, a step-overgrowth process during surface alloy formation, spontaneous stripe formation on Si, and exchange- and vacancy-mediated surface diffusion. We developed new surface probes including the atom-tracking scanning tunneling microscope, spatially resolved LEED-IV analysis, and the pulsed-laser atom-probe.

Program Impact: (1) The IFM is finding broad application in the international research community (17 IFMs in US/Canada). A new concept in IFM-sensor technology promises significant gains in user-friendly operation, sensitivity and speed. (2) Our approach of using engineered defects in controlled oxides to investigate the early stages of pitting allows us to address outstanding questions in corrosion science in a controlled manner. The recent Cu oxidation work clearly shows the importance of near-surface pH changes that can drive corrosion processes. (3) Surface nanostructure research is providing new insights on the microscopic origins of crystal and thin-film growth, surface phase transitions, and surface self-assembly. Over the years, our research has been highlighted in *Science*, *Nature*, *Physics Today*, *Popular Science*, *Popular Mechanics*, *Wall Street Journal*, *MRS Bulletin*, *etc*.

Interactions: Princeton U., U. Houston, U. Minnesota, U. Pittsburgh, Carnegie Mellon, U. Wisconsin at Madison, South Dakota School of Mining and Tech., U. Texas at Austin, U. Western Ontario, Ohio State, North Carolina State, Penn State, Rutgers U., U. of Twente (Netherlands), U. Texas at El Paso, New Mexico State, U. New Mexico, Brookhaven National Labs, Los Alamos National Lab, IBM Yorktown Heights, KFA-Jülich.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Five BES/MS Awards (Houston, Kellogg (2), Feibelman (2), Swartzentruber); 1996 AVS Welch Award (Feibelman); 1997 AVS Peter Mark Award (Swartzentruber); DOE OER's Young Scientist Award (Swartzentruber); 2001 Materials Research Society Medal (Bartelt), 2004 Stanley E. Harrison Faculty Award, OSU (Buchheit); Fellows of the AAAS (Houston), APS (Houston, Feibelman, Kellogg, Bartelt), AVS (Houston, Feibelman, Kellogg, Swartzentruber), numerous editorial boards (PRL, JVST, Prog. in Surf Sci.), conference and symposium organizers, national and international scientific committee positions, and invited talks (>25 in 2004-06).

Personnel Commitments for FY2006 to Nearest +/-10%: (Staff) G. L. Kellogg 40%, J. E. Houston 50%, B. S. Swartzentruber 40%, P. J. Feibelman 70%, W. L. Smith 50%, N. Missert 50%, K. R. Zavadil 50%, J. P. Sullivan 10%, P. Kotula 10%, Ezra Bussmann (post-doc) 100%, N. Vasiljevic (post-doc) 70%, D. Elswick (NSCU grad student) 20%, Y. Kim (OSU grad student) 20%, R. G. Copeland (technologist) 50%.

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA: $1,710 K **FY05 BA:** $1,571 K **FY06 BA:** $ 1,591 K

Laboratory Name: Sandia National Labs / NM
B&R Code: KC 020103

FWP and subtasks under FWP:
FWP – Novel Electronic Materials. Subtasks – 1 Luminescence, Structure, and Growth of Wide-Bandgap Semiconductors; 2 Atomic Processes and Defects in Wide-Bandgap Semiconductors; 3 Field-Structured Anisotropic Composites; and 4 Complex and Cooperative Phenomena in Disordered Ferroelectrics and Dielectrics.

FWP Number: SCW 93222

Program Scope:
We are advancing fundamental understanding of the relation of atomic structure and nanostructure to the interrelated electrical, optoelectronic, ferroelectric, magnetic, and mechanical properties of advanced materials and are developing nanoscale manipulations for property enhancement. Subtasks 1 and 2 elucidate defects, microstructures, and composition fluctuations in GaN and GaInN that alter carrier transport & recombination and luminescence; 3 explores self-assembly in triaxial fields to produce tailored composites with superior magnetic, transport, and mechanical properties; and 4 elucidates cooperative phenomena in disordered quantum ferroelectrics facilitating property optimization. The coordinated application of experiment, first-principles theory, and modeling is central.

Major Program Achievements (over duration of support):

- Our work on group-III-nitrides is enabled by the continuing development of a unique range of capabilities encompassing growth, experimental characterization, density-functional theory, and modeling. (1,2)
- In new subtask 1, we illuminated the carrier behavior underlying luminescence in III-nitride structures by investigating the quantum-confined Stark effect in InGaN/GaN quantum wells. This led to a new model of hole-localization which accounts for anomalous Stark shifts observed in these highly strained structures. Further, we used a novel pulse-recovery technique to determine the transport properties of minority-carrier holes in GaN. (1)
- An integrated effort including experiments, density-functional theory, and modeling yielded quantitative new understanding of the N vacancy (V_N) and N interstitial (N_I) in GaN. This understanding encompasses structure, diffusion, reactions with H and Mg dopants, and their technologically important consequences for p-type doping. Recent achievements include the prediction and experimental detection of the bound complex $MgHN_I$; measurement and prediction of the temperature-dependent diffusivity of N_I; and a predictive model of the device-performance-limiting interplay of dopants, H, and V_N during growth and annealing of p-type GaN. (2)
- We discovered that time-varying, triaxial magnetic fields can synthesize a variety of new particle composites with exceptional properties. Some of these materials enable chemical, pressure, and thermal sensing with extraordinary resolution, *e.g.*, detection of organic vapors at 30 ng/ml. Others exhibit magnetostriction as large as 1% (attractive for actuators); magnetoresistance extending to 10,000,000 % in magnetic fields as low as 0.1 T; and superparamagnetism with specific susceptibilities up to 180 (MKS). These studies include new theoretical models describing the field-influenced dynamics of mixing and structuring. (3)
- In studies of compositionally disordered ABO_3 ferroelectrics, we discovered and elucidated a crossover to a relaxor state with only short-range order, confirmed by the interplay of pressure (favoring the relaxor) and a biasing electric field (promoting long-range order). Our studies of this general phenomenon showed that the relaxor is the ground state at reduced volume; provided insights into static and dynamic properties; and enabled interpretation in terms of the correlation length for dipolar interactions among polar nano-regions. (4)

Program impact:
Increased basic science solid-state lighting, whose potential U.S. energy savings is $ 30 billion per year. (1,2)
Four patents on new field-structured composites with two in preparation. Potential impacts on sensors, actuators. (3)
Breakthrough in understand relaxors, a premier current topic in ferroelectricity with large technological import. (4)
44 publications in 3 years.

Interactions:
In 3 years – 13 universities & research institutions; 3 semiconductor companies.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP):
In 3 years – 15 invited/plenary papers, reviews, & talks; 10 conference & symposium organizations; 1editor.

Personnel Commitments for FY2006 to Nearest +/- 10%:
Myers 20% (FWP lead, 2); Lee 40%, Crawford 20%, Follstaedt 20%, Coltrin 10% (1); Koleske 20% (1,2); Wright 40%, Wampler 10%, [2]; Martin 40%, Read 10%, Huber 10% (3); Venturini 20% (3,4); Samara 30% (4).

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA: $1,571 K **FY05 BA:** $1,450 K **FY06 BA:** $1,388 K

Laboratory Name: Sandia National Labs/NM
B&R Code: KC020105

FWP: Biointegration

FWP Number: SCW 93411

Program Scope: This project involves fundamental materials science studies at the intersection of biology, nanomaterials, and integrated systems. It represents the recent merger of two smaller projects: 1) Active Assembly of Dynamic and Adaptable Materials, which involves learning how to exploit active biomolecules such as motor proteins and microtubules to transport, assemble, and reconfigure nanomaterials, and 2) Artificial Biocompatible Semiconductors for biosystem/material interfaces which involves learning surface functionalization for biocompatibility, processing into micro/nanocavities, and physics of nano-optical transduction for studying biological "soft matter" (biomolecules, pathogens, organelles, and cells) on material surfaces.

Major Program Achievements (over duration of support):
Active Transport of Nanomaterials: Stabilized active proteins (motor proteins and microtubules) have been produced for use in artificial systems via both genetic engineering and chemical crosslinking. Monolayers containing the motor protein kinesin have been used to propel microtubule shuttles plus associated nanoparticle cargo within patterned microfluidic devices. Fundamental nanomechanics studies were performed to understand cargo loading and unloading phenomena, as well as the formation of mobile particle-microtubule composites.
Artificial Microtubule Organizing Centers (AMOCs): 3D constructs consisting of a central functionalized particle, and oriented array of microtubules radiating out from the particle, and molecular motors plus associated cargo have been synthesized. Simulation codes have been developed to model how such constructs can be used to move and assemble nanomaterials via dynamic instability of the microtubules plus motor protein motion, driving experimental efforts to duplicate processes such as diatom assembly and the color changing system of the chameleon.
Biocompatible Semiconductors: A nano-optical transduction method for high-speed spectral analysis of individual nanoparticles (bio- and material particles down to ~100 nm), was discovered. This ultra-sensitive detection of submicron particles uses nano-squeezing of light into photon modes imposed by ultrasmall dimensions in a submicron semiconductor laser cavity. The laser cavity uses high semiconductor gain to trigger the onset of amplification $\sim 10^4$ of a tiny signal from the particle. In effect, the light is "nano-squeezed," through the particle, allowing ultrafast detection and identification.

Program impact: The Active Assembly activity has demonstrated that energy-consuming protein machines can assemble and manipulate materials in new ways that are not limited by diffusion and energy minima constraints encountered in the classical self-assembly of nanomaterials. The project also highlights a new transport mechanism for moving nanomaterials in microfluidic systems that has impacted the development of "on-chip" analysis systems for Homeland Defense (DARPA). The Biocompatible Semiconductors project discovered Nano-Squeezed Light Spectroscopy that has widespread application, including analysis of genetically manipulated yeast mitochondria for high-efficiency ethanol production, detecting biowarfare agents like anthrax spores, and measuring composition and distribution of synthetic organic and inorganic nanoparticles.

Interactions: In addition to co-investigators H. Hess (U. Florida) and V. Vogel (now at ETH, Switzerland), the project has stimulated interactions with R. Haddon (UC Riverside), D. Bear and J. Oliver at the University of New Mexico, and R. K. Naviaux (UC San Diego), K. K. Singh (Roswell Park Institute, NY), and M. F. Gourley (NIH).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
a) 2005 Research Prize, German Phillip Morris Foundation (Hess and Vogel) Symposia Organizer/Chair for 2 MRS Meetings + 2 AAAS Meetings (Bachand and Liu), Cover story in Advanced Functional Materials (1/04) + Invited Review article in Materials Today (in press), Thirteen publications (3 invited) + 12 invited talks. b) ACS Most Highly Accessed Article in *BioTechnology Progress*. (Gourley) Cover Article for Nanotechnology in Biomedicine Journal (Gourley), *APS News* March Meeting top ten news article (Gourley). 7 publications (4 invited talks)

Personnel Commitments for FY2004 to Nearest +/- 10%:
Bunker (35%), Gourley (50%), Bachand (30%), Liu (30%), Osbourn (50%), Sasaki (25%), Hess (20%),Vogel (25%)

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA: $1,401 K **FY05 BA:** $1,381 K **FY06 BA:** $1,197 K

Laboratory Name: Sandia National Laboratories/NM
B&R Code: KC020202

FWP and possible subtask under FWP:
Quantum Electronic Phenomena and Structures
FWP Number: SCW 93220
Program Scope:
In this project we explore quantum electronic and optical properties in MBE or CVD grown and/or lithographically patterned nanoelectronic structures. In detail, the three subtasks that form this project are to study (1) electron-electron interactions in low dimensional systems, (2) the growth and properties of nanostructure arrays and vapor-liquid-solid (VLS) nanowire structures, and (3) transport and coherence in 1D quantum wires and 2D quantum dot superlattices.
Major Program Achievements (over duration of support):
<u>Electron-hole Bilayers:</u> The first completely undoped electron-hole bilayers have been fabricated and studied. Longitudinal and Hall resistance were measured to characterize the bilayers. Recent measurements of Coulomb drag indicate larger than expected drag signatures as has been observed in hole-hole bilayers.
<u>Tunneling and Coulomb drag in double one-dimensional wires:</u> Analysis of tunneling spectroscopy in separately contacted 1D wires shows good agreement with a non-interacting model of electron tunneling. A new device design has been tested to allow both tunneling and Coulomb drag measurements.
<u>Dense, Aligned Arrays of GaN Nanowires:</u> We have demonstrated the growth of dense, highly aligned, single crystalline GaN nanowires on inexpensive r-plane sapphire substrates without the use of patterning or templates. Transmission electron microscopy indicates the [11_20] growth direction.
<u>Hybrid Light-Emitting Devices Based on Colloidal Quantum Dots and InGaN Quantum Wells:</u> We explored a novel approaches for injection of charges into semiconductor nanocrystals by using noncontact pumping mediated by high-efficiency energy transfer (ET) from a proximal quantum well (QW).
<u>Effect of Electron-Electron Scattering on the Conductance of a Quantum Wire:</u> A formalism was developed for calculation of the resistivity in 1D wires. It is observed that the electron-electron (e-e) enhancement is significant while the e-e scattering has no effect in wires where only the ground level is populated.
<u>Valley Degree of Freedom in High Quality Si Quantum Well (QW):</u> A long outstanding problem since 60's, the valley degeneracy in Si was revisited, and first shown to bear many-body origin. Furthermore, we demonstrate that high quality Si QW is an ideal, clean system to study the 2D metal-insulator transition.
<u>Bloch Oscillations and Quantum Transport in 2D Quantum Dot Superlattices:</u> For the first time, evidence of Bloch oscillation was observed in 2D quantum anti-dot arrays, manifested by the edge magnetoplasmon resonance-like behavior and non-linear I-V curve. Evidence of a quantum transition was also observed.
Program impact:
Experiment and theory are combined to discover and understand some of the most exciting physics in quantum nanoelectronics research today. This project synergizes with several other ongoing activities at Sandia, LANL, and UNM, which include high mobility 2D electron layer growth, quantum electron transport, ultra fast optical measurements, and coupled electronic and photonic nanostructures. Moreover, we have built active and fruitful collaborations with outside, well-known scientists, and the resulting work has attracted world-wide attention. We believe that this project will continue to enhance Sandia's position as a leader in the quantum nanoelectronics area.
Interactions:
Collaborations have been established with Princeton (D. Tsui), Caltech (J. Eisenstein), UMD (S. Das Sarma), McGill (G. Gervais), Rice (R. Du), ARL (D. Huang) and the NHMFL. This project has enhanced collaborations between SNL, LANL and the Univ. of New Mexico.
Recognitions, Honors and Awards:
Chairs of EP2DS-16 (Simmons, Lilly); Guest Editor for Physica E (Lilly, Pan, Simmons); V. I. Klimov, LANL Laboratory Fellow (2003); J. A. Simmons, Fellow of the American Physical Society (2002); Invited presentations at the APS March meeting (Reno, 2005; Lilly, 2004; Klimov, 2003; Taylor, 2003), QHSYST06 (Pan), EPQHS05 (Pan, Lilly), LT24 (Pan), PPHMF-5 (Pan), SPIE, 2003 MRS Fall meeting; Invited seminars and colloquia; > 30 publications.
Personnel Commitments for FY2005 to Nearest +/- 10%:
M. P. Lilly (30%), Wei Pan (30%), Ken Lyo (50%), John Reno (20%), Victor Klimov (30%), Toni Taylor (20%), S. Brueck (20%), George Wang (30%)
Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA $1,470K **FY05 BA** $1,190K **FY06 BA** $1,100K

Laboratory Name: Sandia National Labs/NM
B&R Code: KC020301

FWP and possible subtask under FWP: Molecular Nanocomposites
FWP Number: SCW 93223
Program Scope:
This project develops a fundamental understanding of the principles that govern the formation and function of novel nanocomposite materials. The scope of scientific issues being addressed include: 1) the synthesis of robust 2- and 3-D ordered nanocomposite materials with integrated functionalities designed to respond to internal/external stimuli and 2) the required enabling science of complex molecular precursor, nanocluster, and nanoparticle building block synthesis, the understanding of self-assembly mechanisms, and the properties derived from the nanoscale (e.g., transport, electronic, interfacial chemistry, etc.).
Major Program Achievements (over duration of support):
Nanocluster synthesis and characterization: Developed: 1) first room T synthesis of nanocrystalline Si and Ge in high yield with size tunable visible luminesence and 2) cluster surface restructuring to create a white light nanophosphor using a single size semiconductor nanocrystal.
Nanocrystal synthesis: Demonstrated that the structure of precursors used in nanocrystal (NC) synthesis plays a vital role in NC morphology evolution and that molecular design of precursors can be used to control NC morphology for use as building blocks in nanocomposites (e.g. Ge nanodots vs. nanowires).
Molecular assemblies: Developed: 1) new self-assembled monolayers that can be electrochemically programmed in a reversible fashion with specific functional groups and 2) imaging and force measurement techniques that enable the facile characterization of nanoscale chemistry and molecular dynamics in self-organized film and cell surfaces.
Nanostructural architecture and nanocomposites: Work on the formation of gold nanocrystal (NC) micelles and their further self-assembly with soluble silica into three-dimensional gold NC/silica arrays (Fan *et al. Science*, 2004) has been extended to include semiconductor and magnetic NCs with spherical and cubic shapes. Discovered a new nanofabrication approach, cell-directed assembly, in which living cells direct the formation of functional bio/nano interfaces allowing the development of 3D chemical gradients.
Self-assembly: Discovered a new nanofabrication approach, cell-directed assembly, in which living cells direct the formation of functionalbio/nano interfaces allowing the development of 3D chemical gradients.
Nano-assembly characterization: Developed a high-speed ^{1}H and ^{1}H-X nucleus NMR correlation method to probe interactions and domain sizes on the nanoscale in self-assembled materials and used NMR to investigate the phase space and kinetics of magnetically directed self-assembly in CTAB based systems.
Super-hydrophobic surfaces: A novel mechanical re-assembly approach has been developed to produce superhydrophobic silica surfaces using simple procedures like spray or spin coating.

Program impact:
This program has obtained new scientific understanding of the integration of molecular and biomolecular function with nanoscale structures. This new knowledge has led to new internal programs that utilize nanocluster materials in radiation detection, photovoltaics, catalysis, interface control, and taggants. Our enhanced understanding also impacted new projects for NIH, AFOSR, and ARO. The controlled construction of nanoparticles allows exploration of very complex species and architectures to elucidate new and exploitable processes and physics. The new fundamental knowledge of super-hydrophobic surfaces will help in the design of drag reducing coatings.
Interactions: University: 34 profs./24 univs National Lab: LANL/LANL(LANSCE)/LBNL/LLNL
Recognitions, Honors and Awards:
Pubs. in Science, Nature, Nano Letters, Physical Review Letters; JACSMRS Medal (Brinker ’03); DOE’s Lawrence Award (Brinker ’02); MRS Grad. Student Gold Award (Baca ’05); Advisory Board - NIH Center for Biomedical Research (Sasaki); MRS, AVS, and Pacifichem Symp. Organizer (Sasaki, Shreve, Voigt); Ed. Board of *Nanotechnology* (Shelnutt); Rutgers Distinguished Alumnus Award & UNM Regent’s Professor (Brinker ’06); 3 BES awards
Personnel Commitments for FY2006 to Nearest +/- 10%:
T. Boyle (30 %), T. Alam (30%), F. VanSwol (30%), C. J. Brinker (20%), D. Huber (30%), E. Venturini (20%), P. Provencio (20%), H. Fan (20%), A. Burns (20%), B. Bunker (20%), D. Sasaki (20%), J. Shelnutt (20%), J. Voigt (10%).

Authorized Budget (BA) for FY04, FY05, FY06:
FY04 BA: $1,708K **FY05 BA:** $1,665K **FY06 BA:** $1,525K